Non-vanishing spin Hall currents in disordered spin-orbit coupling systems

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Spin-orbit coupling induced spin Hall currents are generic in metals and doped semiconductors. It has recently been argued that the spin Hall conductivity can be dominated by an intrinsic contribution that follows from Bloch state distortion in the presence of an electric field. Here we report on an numerical demonstration of the robustness of this effect in the presence of disorder scattering for the case of a two-dimensional electron-gas with Rashba spin-orbit interactions.

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Semiconductor spintronics research over the past decade has concentrated on the properties of spinpolarized carriers created by optical orientation, on the search for new ferromagnetic semiconductors with more favorable properties, and on the injection of spinpolarized carriers into semiconductors from ferromagnetic metals [1, 2, 3]. There has recently been a flurry of theoretical interest [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23] in the spin Hall effect [4, 5, 6], i.e. in transverse spin currents induced by an electric field. Murakami [7] et al. and Sinova [8] et al. have argued in different contexts that the spin Hall conductivity can be dominated by a contribution that follows from the distortion of Bloch electrons by an electric field and therefore approaches an intrinsic value in the clean limit. This conclusion has recently been questioned, for the case of two-dimensional electrons with Rashba spin-orbit interactions in particular, by several authors [14, 16, 19, 21, 22, 23] motivated by a number of different considerations, some of which are related to controversies [24, 25, 26, 27, 28, 29, 30] that have long surrounded the theory of the anomalous Hall effect in ferromagnetic metals and semiconductors. In this Rapid Communication we report on a study based on numerically exact evaluation of the linear-responsetheory Kubo-formula expression for the spin Hall conductivity. We demonstrate that the intrinsic spin Hall effect is robust in the presence of disorder, falling to zero only when the life-time broadening energy is larger than the spin-orbit splitting of the bands. The correlations between spin-orientation and velocity in the presence of an electric field that lie behind the intrinsic spin Hall effect are not diminished by weak disorder.

We consider a two-dimensional electron system with the Rashba spin-orbit interaction (R2DES):

$$H = \mathbf{p}^2 / 2m + \lambda [\mathbf{p} \times \hat{\mathbf{z}}] \cdot \boldsymbol{\sigma} / \hbar + V. \tag{1}$$

where σ is the Pauli matrix, m is the effective mass, and λ is the Rashba spin-orbit coupling constant. When the disorder potential V in Eq. (1) is absent, $\mathbf{p} = \hbar \mathbf{k}$ is a good quantum number. The Rashba spin-orbit interaction term can be viewed as Zeeman coupling to a

k-dependent effective magnetic field $\Delta = (2\lambda)\hat{\mathbf{z}} \times \mathbf{k}$. The V = 0 eigenstates are therefore the S = 1/2spinors oriented parallel and antiparallel to these fields: $|\mathbf{k}\pm\rangle = [\mp ie^{-i\phi}, 1]e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{2\Omega}$, and the two eigenvalues at a given **k** are split by $2\lambda |\mathbf{k}|$. Here $\phi = \tan^{-1}(k_x/k_y)$, Ω is the system area and we have applied periodic boundary conditions. As explained in Ref. [8], an electric field in the x-direction causes Rashba spinors to tilt out of the x-y plane giving rise to an intrinsic spin Hall effect. The key issue in dispute is whether or not the velocity-dependent spinor tilts vanish when quasiparticle disorder scattering is properly taken into account. To address this subtle issue without making any assumptions which might prejudice the conclusion, we evaluate the Kubo formula for the spin Hall conductivity using the exact single-particle eigenstates of a disordered finite area two-dimensional electron system with Rashba spin-orbit interactions.

Our disorder potential consists of randomly centered scatterers that have strength u_0 and a Gaussian spatial profile with range l_v . The potential matrix elements satisfy $|\langle \mathbf{k}\sigma|V|\mathbf{k}'\sigma'\rangle|^2 = (n_iu_0^2/\Omega)\delta_{\sigma\sigma'}\exp(-|\mathbf{k}-\mathbf{k}'|^2l_v^2)$, where the density of scatterers n_i (intended to represent remote ionized donors) is set equal to the electron density. It is widely recognized that 2DES disorder potentials can have long correlation lengths up to ~ 100 [nm]. To examine how our conclusions depend on the range of the disorder potential, we have performed calculations for correlation lengths ranging from $l_v \sim 0$ to $l_v \sim 100$ [nm].

We diagonalize the Hamiltonian in the $\lambda=0$ eigenstate representation and introduce a hard cutoff at a sufficiently large momentum Λ . For a fixed particle density, the number of electron N_e and the system size are related by $\Omega=L^2=N_e/n_e$. Our conclusions are based on calculations with N_e up to 2258. For $n_e=0.6\times 10^{11}$ [cm⁻²] the system size is up to L=2 [μ m], longer than the characteristic microscopic length scales, the meanfree path $(l\sim 10^2-10^3$ [nm]), the Fermi wavelength $(\lambda_F=2\pi/k_F=101$ [nm]), and the disorder potential range $(l_v\leq 100$ [nm]). The system size in these simulations is comparable to that of typical 2DES channels in electronic devices. We fix the effective mass at the bulk

GaAs value, $m = 0.067m_e$, where m_e is the bare electron mass and perform calculations over a wide range of λ and u_0 values.

The Kubo formula expression for the z spin component of the spin Hall conductivity is:

$$\sigma_{\mu\nu}^{z}(\omega) = \frac{1}{i\Omega} \sum_{n,n'} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}} \frac{\langle n|j_{\mu}^{z}|n'\rangle\langle n'|j_{\nu}|n\rangle}{\hbar\omega + E_n - E_{n'} + i\eta},$$

where f(E) is the Fermi function, n labels exact eigenstates with eigenvalues E_n , and the charge and spin current operators are $\mathbf{j} = -e \ \partial H/\partial \mathbf{p} = -e \ (\mathbf{p}/m + \lambda \hat{\mathbf{z}} \times \boldsymbol{\sigma}/\hbar)$ and $\mathbf{j}^z = \{\partial H/\partial \mathbf{p}, \frac{\hbar}{2}\sigma_z\}/2 = \mathbf{p} \ \sigma_z/m$ respectively [8]. In finite size calculations the electric field turn on time η^{-1} must be shorter than the transit time in the simulation cell in order to obtain the correct thermodynamic limit for the conductivity. In the metallic limit of interest here, η must exceed the simulation cell level spacing but be smaller than all intensive energy scales. In the dc $\omega = 0$ limit, $\sigma^z_{\mu\nu}$ is real with a dissipative contribution that comes from the $i\eta$ term in the denominator and a reactive contribution that comes from the imaginary part of the matrix element product.

Typical numerical results for the disorder and spinorbit coupling strength dependence of the spin Hall conductivity $\sigma_{sH} = \sigma_{xy}^z(\omega = 0)$ are illustrated in Fig.1. (These calculations are for $l_v \sim 80$ [nm].) We find that in the strong Rashba coupling, weak-disorder regime the spin Hall conductivity is close to the (universal) intrinsic value for this model, and that it decreases for weaker spin-orbit coupling and stronger disorder. Experimentally, Rashba spin-orbit coupling strength can be varied over a wide range by tuning a gate field [33, 34]. We have varied the spin-orbit coupling strength at the Fermi energy λk_F from $0.1\epsilon_F$ to $0.4\epsilon_F$. The system size for the calculations summarized by Fig.1 was 1500nm. The range we have chosen for disorder strength values was based on the golden-rule expression for the transport scattering rate[32], $\hbar/\tau = 2\pi \sum_{\mathbf{k'}} |V(\mathbf{k} - \mathbf{k'})|^2 (1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') \delta(\epsilon_{\mathbf{k'}} - \epsilon_F)$. The golden-rule combined with Boltzmann transport theory yields the Drude expression for the longitudinal conductivity, $\sigma_D = ne^2\tau/m = 2\epsilon_F\tau(e^2/h)$. Using these approximate estimates, we have varied the disorder strength so that $\epsilon_F \tau$ covers the range 2 – 20, typical for twodimensional electron systems. For GaAs materials parameters, the disorder strength range that we consider corresponds to mean-free paths l = 70 - 700 [nm]. We note that in the case of short-range scatterers ($l_v \sim 10$ [nm]) the transport lifetime τ defined above is not so different from the momentum lifetime τ_0 given by $\hbar/\tau_0 = 2\pi \sum_{\mathbf{k}'} |V(\mathbf{k} - \mathbf{k}')|^2 \delta(\epsilon_{\mathbf{k}'} - \epsilon_F) \ (l_v \sim 10 \text{ [nm]}), \text{ whereas}$ these quantities differ substantially for longer (and more realistic) correlation lengths. In what follows we take $\hbar = 1$ so that τ^{-1} has energy units. These results demonstrate that for this model σ_{sH} is to reasonable accuracy a function of only $\lambda k_F \tau$, the ratio of the spin-orbit splitting to the quasiparticle state lifetime broadening. The intrinsic spin Hall conductivity survives provided that

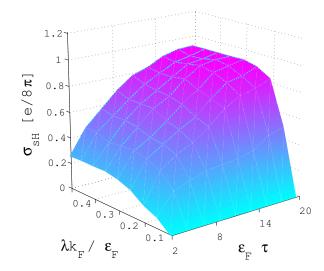


FIG. 1: Spin Hall conductivity σ_{sH} as a function of $\epsilon_F \tau$ and $\lambda k_F/\epsilon_F$ at $\epsilon_F = 2.15$ [meV] and $n_e = 0.6 \times 10^{11}$ [cm⁻²]. For these calculations the system size is L = 1500 [nm] and $l_v = 80$ [nm]. Note that the conductivity depends mainly on $\lambda k_F \tau$ and that, because our interest is limited to the metallic regime, our calculation range does not address the strong scattering limit $\tau \to 0$.

 $\lambda k_F \tau > 1.$

Fig. 2 illustrates some typical system size dependences of the finite-size longitudinal σ_{xx} and spin Hall σ_{sH} conductivities. The size-dependence of transport coefficients in disordered systems can reflect quantum corrections to Boltzmann transport theory due to the interference

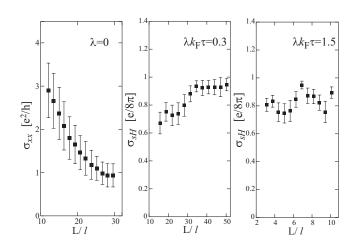


FIG. 2: Left: Size dependence of the longitudinal conductivity σ_{xx} as a function of L/l for $\lambda=0$, $\epsilon_F\tau=2.0$, and $l_v=20$ [nm]; Middle and Right: L/l dependence of the spin Hall conductivity σ_{SH} for $l_v=20$ [nm]) and $\lambda k_F/\epsilon_F=0.3$. The middle panel is for a strongly disordered system in which $\epsilon_F\tau=1$ while the right panel is for the a weakly disordered system in which $\epsilon_F\tau=5$.

effects that cause localization. In two-dimensions, scaling theory and microscopic perturbative calculations predict σ_{xx} corrections that depend on spin-orbit coupling strength and can grow when the system size L is larger than the mean-free path l. The conductivity is expected to decay exponentially with system size in the strongly localized region.[35] Numerical σ_{xx} results for the strongly disordered case $\epsilon_F \tau = 2$, $\lambda = 0$, and $l_v = 20$ [nm], shown in the left panel of Fig.2, are consistent with expectations for this thoroughly studied quantity.[35] Our main interest at present, however, is the system size dependence of the spin Hall conductivity σ_{sH} and particularly in establishing whether or not it vanishes in the limit $L \to \infty$. For σ_{sH} , L should be compared with both l and with the spin-orbit length $L_{so} = l/(\lambda k_F \tau)$. In the middle panel of Fig. [2] $L_{so} \approx 3l$ is the longer intensive length scale, with some system size apparent up to $L/L_{so} \sim 10$. For the more weakly disordered case in the right panel l is longer and no systematic L/l dependence was found. These numerical results appear to establish rather unambiguously that $\lim_{L\to\infty} \sigma_{sH} \neq 0$.

The intrinsic spin Hall effect in the R2DEG is due to a correlation [8] between quasiparticle velocity and the z-component of spin induced by an electric field; for an electric field in the x-direction, an up spin is induced in positive y-component velocity majority-band states and a corresponding down spin at negative velocities. After summing over bands, coherence is confined in momentum space to the annulus of singly-occupied states. These responses are induced by the interband matrix elements of the perturbation term in the Hamiltonian that accounts for the spatially uniform electric field. Since the observable we are interested in here, the spin Hall current, is purely off-diagonal in band indices, its response depends on interband coherence alone and not at all on the altered Bloch state occupation probabilities that dominate most transport coefficients in metals and are the focus of Boltzmann transport theory. If the spin Hall conductivity were to vanish because of disorder scattering, the intrinsic interband coherence would either have to be cancelled at all wavevectors, or be cancelled by stronger coherences induced in a narrow transport window (presumably of width $1/\tau$) centered on the Fermi circles.

In Fig.3 we compare the exact linear-response momentum-dependent z-direction spin-density (and hence interband coherence) for a disorder-free system (left panel) with $\lambda k_F/\epsilon_F = 0.2$ with that of a disordered system (right panel) with the same spin-orbit interaction strength and $\epsilon_F \tau = 3.2$. ($l_v/\lambda_F = 0.2$ for the calculations illustrated in Fig.3.) Both quantities are proportional to the electric field and are plotted in the same units. These results were obtained from the same linear response theory expressions used in Eq.(2) with $S_z(\mathbf{k}) = \sum_{\sigma} \sigma/2 |\mathbf{k}\sigma\rangle\langle\mathbf{k}\sigma| = (|\mathbf{k}+\rangle\langle\mathbf{k}-|+|\mathbf{k}-\rangle\langle\mathbf{k}+|)/2$ substituted for the spin current j_μ^z . The disorder averaged spin Hall conductivity and longitudinal conductivity in this case are $\sigma_{sH}/(e/8\pi) = 0.64$ and $\sigma_{xx}/(e^2/h) = 5.1$ at $\epsilon_F \tau = 3.2$. Our numerical calculations demonstrate

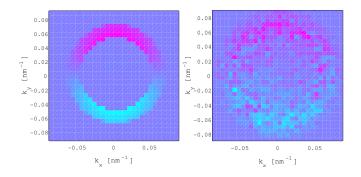


FIG. 3: Electric field induced spin distribution $S_z(\mathbf{k})/eE$ as a function of wave vector for the clean limit (left side) and for an $\epsilon_F \tau = 3.2 \ l_v \lambda_F = 0.2$ disorder model (right side).

that the coherence is not changed qualitatively by impurity scattering, maintaining the same angle dependence as it is spread in momentum space. In particularly there is no evidence that the direction averaged coherence is either cancelled uniformly or cancelled by a strong contribution more narrowly centered on the two Fermi circles.

The subtleties that confuse theories of the spin Hall conductivity in a R2DES are related to issues that arise quite generally in the linear-response theory analysis of non-dissipative transport coefficients, like the anomalous Hall conductivity [37] of a ferromagnet, the ordinary Hall conductivity of a paramagnet, and the spin Hall conductivity of other paramagnetic metals. From an exact eigenstate Kubo formula point of view, these transport coefficients can be dominated by reactive contributions that come from states far from the Fermi level and are not associated with electric field induced level crossings and dissipation. In the spin and anomalous Hall effect cases, the reactive contributions do not vanish in the limit of a perfect crystal, instead approaching an intrinsic value. The currents accounted for by these intrinsic Hall coefficients can be viewed as corresponding to equilibrium currents that flow in an effective periodic systems whose symmetry has been reduced by the electric field. This point has been emphasized recently by Rashba[23], who argues on this basis that the intrinsic response is a transient that will be attenuated within a relaxation time τ scale after the electric field is turned on. Similar arguments have been made concerning the intrinsic contribution to the anomalous Hall effect. [25] The specific instance studied here is perhaps an especially simple example of this class of effects, precisely because $S_z(\mathbf{k})$ and the spin Hall current are purely off-diagonal in band indices. We conjecture, as an extrapolation from the present numerical study, that the part of the density-matrix linear response that is off-diagonal in band index always approaches its intrinsic value in the weak disorder limit. The spin Hall current operator, like the charge current operator in the case of the anomalous Hall effect, will also have intraband matrix elements in the general case. We expect that these can in general lead to extrinsic intraband contributions to the linear response conductivity that remain finite in the weak disorder scattering limit.

In a realistic sample with boundaries, spin density is accumulated at the sample edge by the spin currents. We expect that edge spin accumulations can be measured experimentally. Stevens et al.[36] have recently reported on a remarkable optical measurement of accumulation due to non-linear response spin currents using a spatially resolved pump-probe technique in GaAs/AlGaAs quantum wells. Similar luminescence polarization measurements should be able to detect electrically generated linear response spin Hall currents.

In summary, we calculated the spin Hall conductivity in a disordered system with Rashba spin-orbit coupling using the exactly evaluated eigenstates of the Hamiltonian and the Kubo linear response theory. We find that the field induced spin Hall current of this model approaches its intrinsic value in the limit of weak disorder scattering.

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Note added. —After this work was completed and submitted several preprints appeared reporting on related numerical simulations[38, 39, 40] of spin Hall conductance in finite samples with contacts. These studies reach similar conclusions on the robustness of spin Hall effects. Very recently two experimental preprints[41, 42] have appeared which report detection of edge spin accumulation due to spin Hall currents.

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